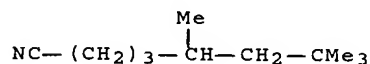


L12 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2004:348009 CAPLUS Full-text  
 DN 140:356957  
 TI Preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation  
 IN Panten, Johannes; Fahlbusch, Karl-Georg; Werner, Matthias; Sillon, Pascal  
 PA Symrise GmbH & Co. KG, Germany  
 SO Eur. Pat. Appl., 7 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA German  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1413570	A1	20040428	EP 2003-22338	20031004
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	DE 10247966	A1	20040506	DE 2002-10247966	20021015
	US 2004127394	A1	20040701	US 2003-684726	20031014
	BR 2003004488	A	20040831	BR 2003-4488	20031014
	JP 2004137275	A2	20040513	JP 2003-354687	20031015
PRAI	DE 2002-10247966	A	20021015		
AB	Fragrant 5,7,7-trimethyloctanenitrile, useful as a fragrance in bleaches, is prepared in high yield and selectivity via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde to give the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octenenitriles which are then subjected to catalytic (e.g., Pd/C) hydrogenation.				
IT	681449-57-0P RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)				
RN	681449-57-0 CAPLUS				
CN	Octanenitrile, 5,7,7-trimethyl- (9CI) (CA INDEX NAME)				



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:876124 CAPLUS Full-text

DN 138:187334

TI Exceptionally long ( $\geq 2.9$  Å) CC bonding interactions in  $\pi$ -[TCNE]<sub>22</sub>- dimers: Two-electron four-center cation-mediated CC bonding interactions involving  $\pi^*$  electrons

AU Del Sesto, Rico E.; Miller, Joel S.; Lafuente, Pilar; Novoa, Juan J.

CS Department of Chemistry, University of Utah, Salt Lake City, UT, 84112-0850, USA

SO Chemistry--A European Journal (2002), 8(21), 4894-4908

CODEN: CEUJED; ISSN: 0947-6539

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

LA English

AB Three groups of singlet ground state [TCNE]<sub>22</sub>- (TCNE = tetracyanoethylene) dimers with characteristic intradimer CC sepsns. (r) and dihedral angles (d) [i.e., group St (r .apprx. 1.6 Å; d = 180°), Lt (r .apprx. 3.5 Å; d = 180°), and Lc (r .apprx. 2.9 Å; d = .apprx. 0°); notation: S/L: short/long bond length; subscript t/c: trans/cis, resp.] are exptl. characterized. The St group is comprised of  $\sigma$ -dimers of [TCNE]•- and octacyanobutanediide, [C<sub>4</sub>(CN)<sub>8</sub>]<sub>2</sub>-, which have a typical, albeit long, sp<sup>3</sup>-sp<sup>3</sup>  $\sigma$  bond (r .apprx. 1.6 Å) between each [TCNE]•- moiety and characteristic  $\nu$ CN,  $\nu$ CC, and  $\delta$ CCN IR absorptions. The L groups are structurally characterized as  $\pi$ -dimers of [TCNE]•- that are either eclipsed with r .apprx. 2.9 Å (Lc) and the nitriles bend away from the nominal TCNE plane away from the center of the dimer by 5.0° (.apprx.sp2.17) or are noneclipsed with r .apprx. 3.5 Å (Lt) and the nitriles bend toward the center of the dimer by 1.9° (.apprx.sp2.06). Ab initio computations on isolated dimers were used to study the formation and stability of these exceptionally long CC ( $\geq 2.9$  Å) bonding interactions as well as the process of  $\pi$ -[TCNE]<sub>22</sub>- dimer formation for the Lc and Lt groups. The results of these computational studies show that the ground-state potential curve is that of a closed-shell/open-shell singlet, depending on the distance. The short St group (r .apprx. 1.6 Å) of dimers in this surface are true min.-energy structures; however, the Lt and Lc groups are unstable, although two different nonphys. min. are found when imposing a double occupancy of the orbitals. These min. are metastable relative to dissociation into the isolated [TCNE]•- units. Consequently, the existence of dimer dianions in crystals is due to cation ... [TCNE]- interactions, which provide the electrostatic stabilization necessary to overcome the intradimer electrostatic repulsion. This cation-mediated  $\pi^*$ - $\pi^*$  [TCNE]- ... [TCNE]- interaction complies with Pauling's definition of a chemical bond. This bonding interaction involves the  $\pi^*$  orbitals of each fragment, and arise from the overlap of the b<sub>2g</sub> SOMO on each of the two [TCNE]•-s to form a filled b<sub>2u</sub> [TCNE]<sub>22</sub>- orbital. Although a  $\pi$  dimer typically forms, if the fragments are close enough a  $\sigma$  dimer can form. Due to the presence of cation-mediated intradimer CC bonding interactions the Lc group of  $\pi$ -[TCNE]<sub>22</sub>- dimers exhibits exptl. observable  $\nu$ CN IR absorptions at 2191  $\pm$  2 (m), 2173  $\pm$  3 (s), and 2162  $\pm$  3 cm<sup>-1</sup> (s) and  $\nu$ CC at 1364  $\pm$  3 cm<sup>-1</sup> (s) as well as a new UV-Vis feature in the range of 15000 to 18200 cm<sup>-1</sup> (549 to 667 nm) and averaging 16825  $\pm$  1180 cm<sup>-1</sup> (594 nm) assigned to the predicted new intradimer 1A<sub>1g</sub>  $\rightarrow$  1B<sub>1u</sub> transition and is purple on reflected light. Upon cooling to 77 K in 2-methyltetrahydrofuran, this

new band occurs at 18940 cm<sup>-1</sup> (528 nm) for { [Et<sub>4</sub>N]<sup>+</sup> }<sub>2</sub> [TCNE]<sub>22</sub><sup>-</sup>, and the yellow solution turns deep red. Group Lt is characterized by vCN absorptions at 2215 ± 2, 2197 ± 3, and 2180 ± 4 cm<sup>-1</sup> and vCC at 1209 ± 9 cm<sup>-1</sup> (w), while group ST has vCN bands at 2215 ± 4, 2157 ± 3, and 2107 ± 4 cm<sup>-1</sup> and vCC at 1385 ± 1 cm<sup>-1</sup> (vs).

IT 210233-00-4

RL: PRP (Properties)

(exceptionally long CC bonding interactions in π-[TCNE]<sub>22</sub><sup>-</sup> dimers with two-electron four-center cation-mediated CC bonding interactions involving π\* electrons)

RN 210233-00-4 CAPLUS

CN Iron(2+), bis(acetonitrile)-, salt with 1,1,2,2,3,3,4,4-butaneeoctacarbonitrile, compd. with acetonitrile (1:1:1) (9CI) (CA

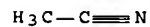
INDEX

NAME)

CM 1

CRN 75-05-8

CMF C2 H3 N



CM 2

CRN 210232-99-8

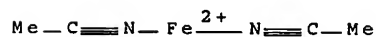
CMF C12 N8 . C4 H6 Fe N2

CM 3

CRN 210232-98-7

CMF C4 H6 Fe N2

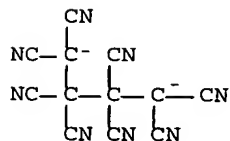
CCI CCS



CM 4

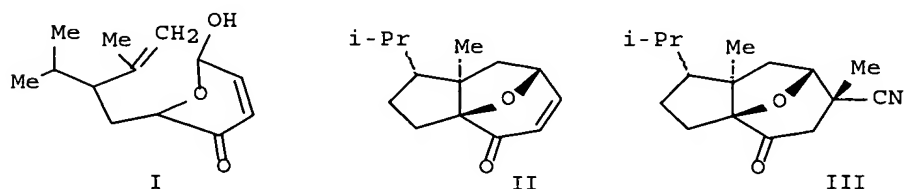
CRN 210232-94-3

CMF C12 N8



RE.CNT 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2001:498880 CAPLUS Full-text  
 DN 135:304028  
 TI Stereoselective synthesis of the bicyclo[5.3.0]decane portion of the  
 diterpene antibiotic guanacastepene using a pyrylium-ylide [5+2]  
 cycloaddition reaction  
 AU Magnus, P.; Waring, M. J.; Ollivier, C.; Lynch, V.  
 CS Department of Chemistry and Biochemistry, University of Texas at Austin,  
 Austin, TX, 78712, USA  
 SO Tetrahedron Letters (2001), 42(30), 4947-4950  
 CODEN: TELEAY; ISSN: 0040-4039  
 PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 OS CASREACT 135:304028  
 GI



AB Treatment of I with Ac<sub>2</sub>O/Et<sub>3</sub>N resulted in [5+2] cyclization to give II,  
 which was further elaborated into III, thus establishing the required  
 stereochem. in the top-half of guanacastepene.

IT 365978-34-3P 365978-53-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

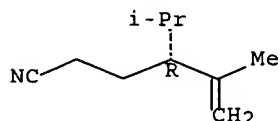
(Reactant or reagent)

(stereoselective synthesis of bicyclo[5.3.0]decane portion of  
 diterpene  
 antibiotic guanacastepene using a pyrylium-ylide [5+2] cycloaddn.  
 reaction)

RN 365978-34-3 CAPLUS

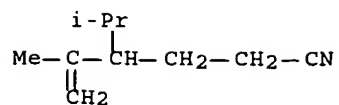
CN 5-Hexenenitrile, 5-methyl-4-(1-methylethyl)-, (4R)- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry. Rotation (+).



RN 365978-53-6 CAPLUS

CN 5-Hexenenitrile, 5-methyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



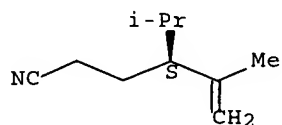
IT 365978-51-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (stereoselective synthesis of bicyclo[5.3.0]decane portion of  
 diterpene  
 antibiotic guanacastepene using a pyrylium-ylide [5+2] cycloaddn.  
 reaction)

RN 365978-51-4 CAPLUS

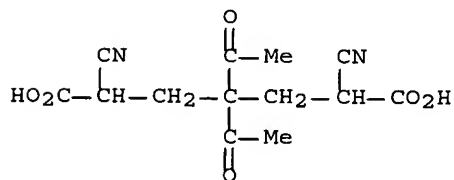
CN 5-Hexenenitrile, 5-methyl-4-(1-methylethyl)-, (4S)- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry. Rotation (-).

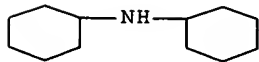


RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 2000:148131 CAPLUS Full-text  
 DN 132:278725  
 TI Self-catalytic Michael reaction. An efficient route to 2-cyanoalkanoic acids  
 AU Krawczyk, Henryk  
 CS Institute of Organic Chemistry, Technical University (Politechnika), Lodz, 90924, Pol.  
 SO Synthetic Communications (2000), 30(4), 657-664  
 CODEN: SYNCAV; ISSN: 0039-7911  
 PB Marcel Dekker, Inc.  
 DT Journal  
 LA English  
 OS CASREACT 132:278725  
 AB The self-catalytic Michael reaction of several 1,3-dicarbonyl compds. with dicyclohexylammonium 2-cyanoacrylate proceeded highly efficiently at room temperature to give the corresponding 1,4-adducts.  
 IT 263703-46-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (self-catalytic Michael reaction in preparation of 2-cyanoalkanoic acids)  
 RN 263703-46-4 CAPLUS  
 CN Heptanedioic acid, 4,4-diacetyl-2,6-dicyano-, compd. with N-cyclohexylcyclohexanamine (1:2) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 263703-45-3  
 CMF C13 H14 N2 O6

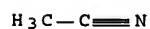


CM 2  
 CRN 101-83-7  
 CMF C12 H23 N

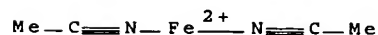


RE.CNT 8      THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1998:433463 CAPLUS Full-text  
 DN 129:130514  
 TI Isolation and structural determination of octacyanobutanediide,  
 [C<sub>4</sub>(CN)<sub>8</sub>]<sup>2-</sup>; precursors to M(TCNE)<sub>x</sub> magnets  
 AU Zhang, Jie; Del Sesto, Rico E.; Gordon, Douglas C.; Miller, Joel S.;  
 Zhang, Jie; Liable-Sands, Louise M.; Rheingold, Arnold L.; Burkhardt,  
 Brian  
 M.  
 CS Department of Chemistry, University of Utah, Salt Lake City, UT,  
 84112-0850, USA  
 SO Chemical Communications (Cambridge) (1998), (13), 1385-1386  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PB Royal Society of Chemistry  
 DT Journal  
 LA English  
 AB The reaction of M<sub>2</sub>·xMeCN (M = Mn, Fe) and TCNE (tetracyanoethylene)  
 leads to unprecedented [C<sub>4</sub>(CN)<sub>8</sub>]<sup>2-</sup> μ<sub>4</sub>-metal complexes which were  
 crystallog. characterized and are precursors to M(TCNE)<sub>x</sub>·yS magnets.  
 IT 210233-00-4P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation, crystal structure of polymeric μ<sub>4</sub>-octacyanobutanediide  
 complex, and thermal decomposition to give metal TCNE magnet)  
 RN 210233-00-4 CAPLUS  
 CN Iron(2+), bis(acetonitrile)-, salt with 1,1,2,2,3,3,4,4-  
 butaneoctacarbonitrile, compd. with acetonitrile (1:1:1) (9CI) (CA  
 INDEX  
 NAME)  
 CM 1  
 CRN 75-05-8  
 CMF C2 H3 N



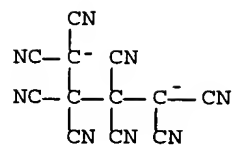
CM 2  
 CRN 210232-99-8  
 CMF C12 N8 . C4 H6 Fe N2  
 CM 3  
 CRN 210232-98-7  
 CMF C4 H6 Fe N2  
 CCI CCS



CM 4

CRN 210232-94-3

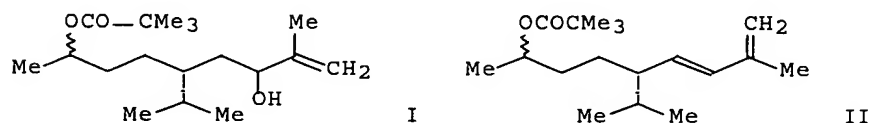
CMF C12 N8



RE.CNT 22      THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

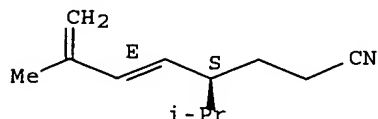


L12 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1994:604511 CAPLUS Full-text  
 DN 121:204511  
 TI Facile preparation of conjugated dienes from allylic alcohols  
 AU Kitahara, Takeshi; Matsuoka, Tatsuji; Kiyota, Hiromasa; Warita, Yasuhiro;  
 Kurata, Hitoshi; Horiguchi, Akira; Mori, Kenji  
 CS Department of Agricultural Chemistry, University of Tokyo, Tokyo, 113, Japan  
 SO Synthesis (1994), (7), 692-4  
 CODEN: SYNTBF; ISSN: 0039-7881  
 DT Journal  
 LA English  
 OS CASREACT 121:204511  
 GI



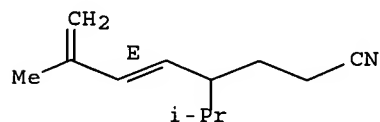
AB An efficient two-step procedure to prepare conjugated dienes from allylic alcs. is developed without the formation of regioisomers and rearranged products. Thus, to a solution of I and dry Et<sub>3</sub>N in dry CH<sub>2</sub>Cl<sub>2</sub> was added dropwise methanesulfonyl chloride; after workup, the crude mesylate was dissolved in diisopropylethylamine (Hunig's base) and dry HMPA and heated at 160° for 20 min. to give (2R,5R)-8-methyl-5-(1-methylethyl)-6,8-nonadien-2-yl pivalate (II) in 64% yield.  
 IT 157905-12-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 157905-12-9 CAPLUS  
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, [S-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



L12 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1994:134846 CAPLUS Full-text  
 DN 120:134846  
 TI A new synthesis of solanone  
 AU Park, Oee Sook; Kim, Hong Jin; Chae, Woo Ki; Lee, Woo Young  
 CS Dep. Chem., Chungbuk Natl. Univ., Chungbuk, 306-763, S. Korea  
 SO Bulletin of the Korean Chemical Society (1993), 14(5), 639-41  
 CODEN: BKCSDE; ISSN: 0253-2964  
 DT Journal  
 LA English  
 OS CASREACT 120:134846  
 AB A new synthesis of solanone, (E)-MeCOCH<sub>2</sub>CH<sub>2</sub>CH(CHMe<sub>2</sub>)CH:CHCMe:CH<sub>2</sub>,  
 suitable for use in the perfume industry, is described. Et isovalerate  
 or di-Me malonate are the readily available starting materials.  
 IT 51513-11-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (intermediate in preparation of solanone from isovalerate or  
 malonate)  
 RN 51513-11-2 CAPLUS  
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, (E)- (9CI) (CA INDEX  
 NAME)

Double bond geometry as shown.



L12 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1994:129084 CAPLUS Full-text  
 DN 120:129084  
 TI Polyacrylonitrile modified with hydrogen halide for immobilization of biological substances  
 IN Howard, Edward G., Jr.; Shannon, Patrick T.  
 PA du Pont de Nemours, E. I., and Co., USA  
 SO U.S., 7 pp. Cont. of U.S. Ser. No. 641,991, abandoned.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	US 5262317	A	19931116	US 1992-939567	19920903
PRAI	US 1988-275189	B1	19881123		
	US 1991-641991	B1	19910116		

AB Polyacrylonitrile is chemical modified with HX (X = Cl, Br, I, CF<sub>3</sub>SO<sub>3</sub>) to produce a polymer with readily replaceable X groups. The modified polyacrylonitrile is useful as an immobilization substrate for, e.g., proteins and in affinity chromatog. Preparation of the halo-modified polyacrylonitriles is included. Immobilization of an anti-apoprotein B monoclonal antibody and of Staphylococcus aureus-derived protein A is described.

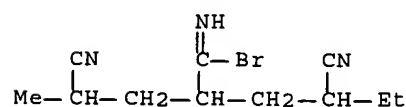
IT 153087-08-2 153087-12-8 153087-16-2  
 153087-20-8  
 RL: ANST (Analytical study)  
 (for biol. material immobilization)

RN 153087-08-2 CAPLUS

CN Hexanimidoyl bromide, 4-cyano-2-(2-cyanopropyl)-, polymer with 2-propenenitrile (9CI) (CA INDEX NAME)

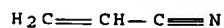
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CRN 153087-07-1  
 CMF C11 H16 Br N3



CM 2

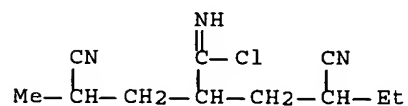
CRN 107-13-1  
 CMF C3 H3 N



RN 153087-12-8 CAPLUS  
CN Hexanimidoyl chloride, 4-cyano-2-(2-cyanopropyl)-, polymer with  
2-propenenitrile (9CI) (CA INDEX NAME)

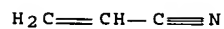
CM 1

CRN 153087-11-7  
CMF C11 H16 Cl N3



CM 2

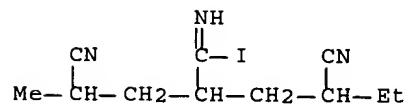
CRN 107-13-1  
CMF C3 H3 N



RN 153087-16-2 CAPLUS  
CN Hexanimidoyl iodide, 4-cyano-2-(2-cyanopropyl)-, polymer with  
2-propenenitrile (9CI) (CA INDEX NAME)

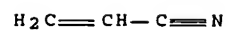
CM 1

CRN 153087-15-1  
CMF C11 H16 I N3



CM 2

CRN 107-13-1  
CMF C3 H3 N



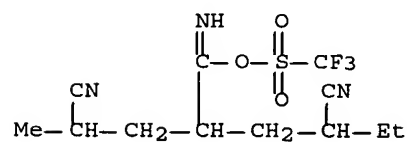
RN 153087-20-8 CAPLUS

CN Hexanimidic acid, 4-cyano-2-(2-cyanopropyl)-, anhydride with trifluoromethanesulfonic acid, polymer with 2-propenenitrile (9CI) (CA INDEX NAME)

CM 1

CRN 153087-19-5

CMF C12 H16 F3 N3 O3 S



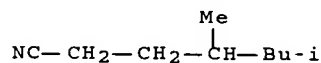
CM 2

CRN 107-13-1

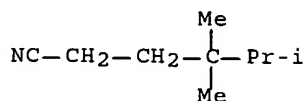
CMF C3 H3 N



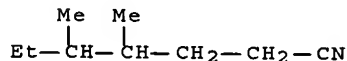
L12 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1992:160132 CAPLUS Full-text  
 DN 116:160132  
 TI Thermochemical parameters of nitriles in the ideal gas state  
 AU Bures, Michal; Cerny, Cestmir; Holub, Robert  
 CS Vys. Sk. Chemickotechnol., Prague, Czech.  
 SO Chemicky Prumysl (1990), 40(11-12), 589-95  
 CODEN: CHPUA4; ISSN: 0009-2789  
 DT Journal  
 LA Czech  
 AB The functional group contribution approach was used to derive the parameters of the equations for the calcn. of the heat capacities and free energy functions of alkyl nitriles (C5-C9). The values of these parameters for compds. are tabulated.  
 IT 78695-45-1, 4,6-Dimethylheptanonitrile 99064-65-0, 4,4,5-Trimethylhexanonitrile 138807-85-9, 4,5-Dimethylheptanonitrile 138807-91-7, 5,6-Dimethylheptanonitrile 138807-97-3, 3,4,5-Trimethylhexanonitrile 138808-02-3, 2,4,5-Trimethylhexanonitrile 138808-04-5, 4,5,5-Trimethylhexanonitrile 138808-14-7, 4-Ethyl-5-methylhexanonitrile 138808-42-1, 4,5-Dimethylhexanonitrile  
 RL: PRP (Properties)  
 (free energy function and heat capacity equations for, parameters for, in ideal gas state)  
 RN 78695-45-1 CAPLUS  
 CN Heptanenitrile, 4,6-dimethyl- (9CI) (CA INDEX NAME)



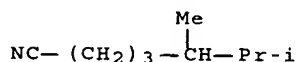
RN 99064-65-0 CAPLUS  
 CN Hexanenitrile, 4,4,5-trimethyl- (9CI) (CA INDEX NAME)



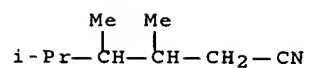
RN 138807-85-9 CAPLUS  
 CN Heptanenitrile, 4,5-dimethyl- (9CI) (CA INDEX NAME)



RN 138807-91-7 CAPLUS  
 CN Heptanenitrile, 5,6-dimethyl- (9CI) (CA INDEX NAME)

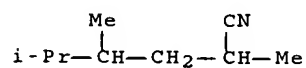


RN 138807-97-3 CAPLUS  
 CN Hexanenitrile, 3,4,5-trimethyl- (9CI) (CA INDEX NAME)



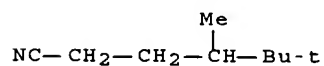
RN 138808-02-3 CAPLUS

CN Hexanenitrile, 2,4,5-trimethyl- (9CI) (CA INDEX NAME)



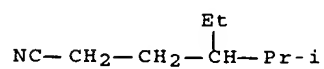
RN 138808-04-5 CAPLUS

CN Hexanenitrile, 4,5,5-trimethyl- (9CI) (CA INDEX NAME)



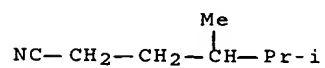
RN 138808-14-7 CAPLUS

CN Hexanenitrile, 4-ethyl-5-methyl- (9CI) (CA INDEX NAME)

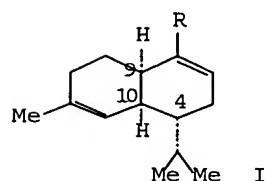


RN 138808-42-1 CAPLUS

CN Hexanenitrile, 4,5-dimethyl- (9CI) (CA INDEX NAME)

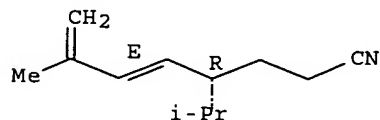


L12 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1987:5248 CAPLUS Full-text  
 DN 106:5248  
 TI Synthetic microbial chemistry. XII. Synthesis of both enantiomers of sclerosporin and sclerosporal, sporogenic substances of *Sclerotinia fructicola*  
 AU Kitahara, Takeshi; Kurata, Hitoshi; Matsuoka, Tatsuji; Mori, Kenji  
 CS Dep. Agric. Chem., Univ. Tokyo, Tokyo, 113, Japan  
 SO Tetrahedron (1985), 41(23), 5475-85  
 CODEN: TETRAB; ISSN: 0040-4020  
 DT Journal  
 LA English  
 OS CASREACT 106:5248  
 GI



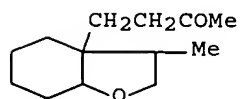
AB Both enantiomers of sclerosporin and sclerosporal were synthesized from (-)-carvone. (4R,9R,10S)-(+)-Sclerosporin (I, R = CO<sub>2</sub>H) and (4R,9R,10S)-(-)-sclerosporal (I, R = CHO) were identified as the natural enantiomers by a comparison of their CD spectra. An intramol. Diels-Alder route proved to be an efficient method of preparing sufficient amts. of I for future biol. study.  
 IT 105661-26-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as intermediate for sclerosporin)  
 RN 105661-26-5 CAPLUS  
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, [R-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



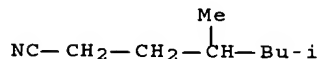


L12 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1986:405818 CAPLUS Full-text  
 DN 105:5818  
 TI Denitrohydrogenation of aliphatic nitro compounds and a new use of  
 aliphatic nitro compounds as radical precursors  
 AU Ono, Noboru; Miyake, Hideyoshi; Kamimura, Akio; Hamamoto, Isami; Tamura,  
 Rui; Kaji, Aritsune  
 CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan  
 SO Tetrahedron (1985), 41(19), 4013-23  
 CODEN: TETRAB; ISSN: 0040-4020  
 DT Journal  
 LA English  
 OS CASREACT 105:5818  
 GI

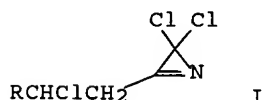


I

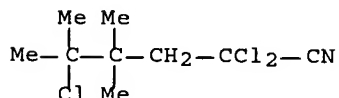
AB Denitrohydrogenation of  $RR_1R_2CNO_2$  ( $R-R_2$  = alkyl, aryl) by  $Bu_3SnH$  in  $C_6H_6$   
 in the presence of AIBN gave  $RR_1R_2CH$ . Compds. activated by CN, COR, or  
 $CO_2R$  groups, e.g.,  $PhCOCMe_2NO_2$ , were readily denitrohydrogenated.  
 Presence of radical leaving groups gave elimination reactions in some  
 cases; thus, treating  $PhCH(NO_2)CH(SPh)Ph$  with  $Bu_3SnH$  gave only E-  
 $PhCH:CHPh$ , with no product resulting from denitrohydrogenation. The  
 radical intermediates generated by denitration were also used in C-C:  
 reforming reactions, e.g., cyclization. Thus, treating  
 (allyloxy)nitrocyclohexane with  $Bu_3SnH$  gave a high yield of the furan  
 derivative I. Also used as the C-C bond-forming reaction was the  
 intermol. addition of radicals to alkenes.  
 IT 78695-45-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by denitrohydrogenation of nitroalkane)  
 RN 78695-45-1 CAPLUS  
 CN Heptanenitrile, 4,6-dimethyl- (9CI) (CA INDEX NAME)



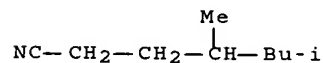
L12 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1985:504806 CAPLUS Full-text  
 DN 103:104806  
 TI The Prins-type reactions of mono- and 1,1-disubstituted alkenes with trichloroacetonitrile in the presence of boron trichloride  
 AU Hamana, Hiroshi; Sugasawa, Tsutomu  
 CS Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan  
 SO Chemistry Letters (1985), (5), 571-4  
 CODEN: CMLTAG; ISSN: 0366-7022  
 DT Journal  
 LA English  
 OS CASREACT 103:104806  
 GI



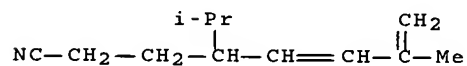
AB BCl<sub>3</sub> catalyzed the Prins-type reaction of alkenes RCH:CH<sub>2</sub> (R = hexyl, Bu, Me<sub>2</sub>CHCH<sub>2</sub>, EtCHMe, Me<sub>3</sub>C, PhCH<sub>2</sub>) with Cl<sub>3</sub>CCN to give dichloroazirines I in high yields. Further exposure of I to BCl<sub>3</sub> at room temperature afforded RCHClCH<sub>2</sub>CCl<sub>2</sub>CN. The Prins-type acylations of R<sub>1</sub>R<sub>2</sub>C:CH<sub>2</sub> [R<sub>1</sub>R<sub>2</sub> = (CH<sub>2</sub>)<sub>5</sub>, (CH<sub>2</sub>)<sub>3</sub>; R<sub>1</sub> = R<sub>2</sub> = Et; R<sub>1</sub> = CMe<sub>3</sub>, CHMe<sub>2</sub>, R<sub>2</sub> = Me], limonene, and camphene with Cl<sub>3</sub>CCN gave R<sub>1</sub>R<sub>2</sub>CClCH<sub>2</sub>COC<sub>2</sub>Cl<sub>3</sub> and R<sub>1</sub>R<sub>2</sub>C:CHCOC<sub>2</sub>Cl<sub>3</sub>.  
 IT 97963-01-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 97963-01-4 CAPLUS  
 CN Hexanenitrile, 2,2,5-trichloro-4,4,5-trimethyl- (9CI) (CA INDEX NAME)



L12 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1981:496925 CAPLUS Full-text  
 DN 95:96925  
 TI A new synthetic method: direct replacement of the nitro group by  
 hydrogen  
 or deuterium  
 AU Ono, Noboru; Miyake, Hideyoshi; Tamura, Rui; Kaji, Aritsune  
 CS Dep. Chem., Kyoto Univ., Kyoto, 606, Japan  
 SO Tetrahedron Letters (1981), 22(18), 1705-8  
 CODEN: TELEAY; ISSN: 0040-4039  
 DT Journal  
 LA English  
 OS CASREACT 95:96925  
 AB Bu<sub>3</sub>SnR(R = H, D) denitrate tertiary or secondary aliphatic and aryl  
 nitro compds. to give the corresponding alkanes or deuterioalkanes.  
 Thus, treatment of Me<sub>3</sub>CCH<sub>2</sub>CMe<sub>2</sub>NO<sub>2</sub> with Bu<sub>3</sub>SnH in refluxing C<sub>6</sub>H<sub>6</sub> in the  
 presence of AIBN for 2 h gave 75 % Me<sub>3</sub>CCH<sub>2</sub>CHMe<sub>2</sub>. Similarly, treatment  
 of 4-NCC<sub>6</sub>H<sub>4</sub>CMe<sub>2</sub>NO<sub>2</sub> with Bu<sub>3</sub>SnD in C<sub>6</sub>H<sub>6</sub>-AIBN for 1.5 h gave 85% 4-  
 NCC<sub>6</sub>H<sub>4</sub>CDMe<sub>2</sub>.  
 IT 78695-45-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by denitration reaction)  
 RN 78695-45-1 CAPLUS  
 CN Heptanenitrile, 4,6-dimethyl- (9CI) (CA INDEX NAME)

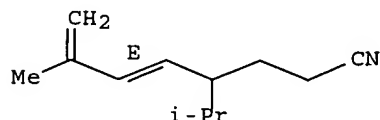


L12 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1979:439653 CAPLUS Full-text  
 DN 91:39653  
 TI Synthesis of methyl 4-isopropyl-7-methyl-5,7-octadienoate  
 AU Watanabe, Shoji; Fujita, Tsutomu; Suga, Kyoichi; Inaba, Teruhiko;  
 Tsuruta,  
 Haruki  
 CS Fac. Eng., Chiba Univ., Chiba, Japan  
 SO Yukagaku (1979), 28(2), 115-16  
 CODEN: YK GKAM; ISSN: 0513-398X  
 DT Journal  
 LA Japanese  
 OS CASREACT 91:39653  
 AB Analogs of solanone were prepared Condensation of Me<sub>2</sub>CHCH<sub>2</sub>CHO  
 piperidine enamine with CH<sub>2</sub>:CHCO<sub>2</sub>Me and CH<sub>2</sub>:CHCN gave  
 RCH<sub>2</sub>CH<sub>2</sub>CH(CHMe<sub>2</sub>)CHO [R = CO<sub>2</sub>Me (I) and CN (II); resp.]. Wittig reaction  
 of I with CH<sub>2</sub>:CMeCH:PPh<sub>3</sub> in THF gave H<sub>2</sub>C:CMeCH:CHCH(CHMe<sub>2</sub>)CH<sub>2</sub>CH<sub>2</sub>R<sub>1</sub> (III;  
 R<sub>1</sub> = CO<sub>2</sub>Me). Similarly II gave III (R<sub>1</sub> = CN), hydrolysis of which under  
 basic condition gave cis- and trans-Me<sub>2</sub>C:CHCH:C(CHMe<sub>2</sub>)CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Me.  
 IT 70687-52-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT  
 (Reactant or reagent)  
 (preparation and hydrolysis of)  
 RN 70687-52-4 CAPLUS  
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

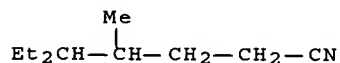


L12 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1978:538029 CAPLUS Full-text  
 DN 89:138029  
 TI Nuclear magnetic resonance study of metal complexes. 2. Conformations  
 of  
 1,2-diamine chelate rings with C-phenyl group(s) in cobalt(III) and  
 platinum(II) complexes  
 AU Yano, S.; Tukada, T.; Saburi, M.; Yoshikawa, S.  
 CS Fac. Eng., Univ. Tokyo, Tokyo, Japan  
 SO Inorganic Chemistry (1978), 17(9), 2520-6  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DT Journal  
 LA English  
 AB The proton NMR spectra of [Co(CN)<sub>4</sub>(R-phenyl)] (R- phenyl = R-  
 phenylethylenediamine), [Pt(NH<sub>3</sub>)<sub>2</sub>(pn-d1)]<sup>2+</sup> (pn-d1 = 2-deuterio-1,2-  
 aminopropane), [Pt(S-pn-d2)<sub>2</sub>]<sup>2+</sup> (S-pn-d2 = (2S)-1,1-dideuterio-1,2,-  
 aminopropane), [Pt(S,S-bn)<sub>2</sub>]<sup>2+</sup> (S,S-n = (2S,3S)-2,3-butanediamine  
 [Pt(en)((-)-D-stien)]<sup>2+</sup> ((-)-1D-stien = silbenediamine) were measured for  
 the diamine chelates with C-Ph group(s) a Karplus-like dihedral angle  
 dependence for the JPt-N-C-C+, where C+ is a Ph atom which attaches on  
 the membered-C atom, was observed These 3JPt-C+ values were very  
 similar to those for the JPt-N-C-CH<sub>3</sub> in the diamine chelates with C-Me  
 group(s).  
 IT 51513-11-2  
 RL: PRP (Properties)  
 (NMR and conformation of)  
 RN 51513-11-2 CAPLUS  
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, (E)- (9CI) (CA INDEX  
 NAME)

Double bond geometry as shown.

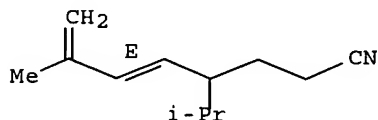


L12 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1976:433624 CAPLUS Full-text  
 DN 85:33624  
 TI Functionalization of unsaturated polymers. Action of chloroacetonitrile  
 in basic media on polyalkadiene organoborane derivatives  
 AU Pinazzi, C. P.; Vassort, J.; Noireaux, P.; Reyx, D.  
 CS Lab. Chim. Org. Macromol., Cent. Univ., Le Mans, Fr.  
 SO European Polymer Journal (1976), 12(2), 83-6  
 CODEN: EUPJAG; ISSN: 0014-3057  
 DT Journal  
 LA French  
 AB Poly(1,2-butadiene), poly(1,4-butadiene) [9003-17-2], poly(3,4-isoprene)  
 [9003-31-0], and poly(1,4-isoprene) and models of their structural  
 repeating units, i.e. 3-ethylpentene [4038-04-4], 4-octene [592-99-4],  
 3-ethyl-2-methylpentene [19780-66-6], and 4-methyl-4-octene [38304-63-1]  
 were treated with 9-borabicyclononane [25301-61-5] and then with K tert-  
 butylphenoxide and ClCH<sub>2</sub>CN. The monomers gave 65-84% yields of products  
 with the cyanomethyl groups attached to the least substituted C and  
 cyanomethylated polymer yields were 60-82% depending on microstructure.  
 IT 59333-88-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 59333-88-9 CAPLUS  
 CN Heptanenitrile, 5-ethyl-4-methyl- (9CI) (CA INDEX NAME)



L12 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1974:45798 CAPLUS Full-text  
 DN 80:45798  
 TI Tobacco chemistry. 20. Structures and syntheses of three new tobacco constituents of probable isoprenoid origin  
 AU Aasen, Arne J.; Hlubucek, Joseph R.; Almqvist, Sven; Kimland, Bjarne; Enzell, Curt R.  
 CS Res. Dep., Swed. Tob. Co., Stockholm, Swed.  
 SO Acta Chemica Scandinavica (1947-1973) (1973), 27(7), 2405-10  
 CODEN: ACSAA4; ISSN: 0001-5393  
 DT Journal  
 LA English  
 AB The structures of 3 new tobacco isolates, 5ξ-isopropyl-3E-hepten-2-one, 3ξ-hydroxy-3ξ-methyl-6ξ-isopropyl-4E-octenoic acid, and 2,10-dimethyl-7ξ-isopropyl-8E-10-undecadien-4-one have been elucidated on the basis of their spectral data and subsequently confirmed by total syntheses. The possible isoprenoid origin of these compds. is discussed.  
 IT 51513-11-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with isobutylmagnesium bromide)  
 RN 51513-11-2 CAPLUS  
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L12 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1965:438851 CAPLUS Full-text

DN 63:38851

OREF 63:6913e-h

TI Reduction of aromatic and branched-chain aliphatic nitriles by SnCl<sub>2</sub>  
(Stephen aldehyde synthesis)

AU Pyryalova, P. S.; Zil'berman, E. N.

SO Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya  
Tekhnologiya (1965), 8(1), 82-7  
CODEN: IVUKAR; ISSN: 0579-2991

DT Journal

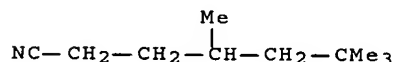
LA Russian

AB The Stephen aldehyde synthesis, reduction of nitriles by treatment with anhydrous SnCl<sub>2</sub> dissolved in Et<sub>2</sub>O saturated with HCl and subsequent hydrolysis of the aldimines formed, was investigated for determination of optimum reaction conditions. Using PhCN, the following factors were found to influence the yield of BzH: (1) the Et<sub>2</sub>O solution of PhCN should be saturated with HCl gas and the resulting mixture kept 3-4 hrs.; (2) the reaction temperature should be 20° (89% yield BzH) rather than 0° (85%); (3) the molar ratio RCN-SnCl<sub>2</sub> of 1:2 (100%) instead of 1:1.1 (74%); (4) a stream of HCl gas should be conducted through the combined solns. of RCN and SnCl<sub>2</sub> until the solution is homogeneous; precipitation of the aldimine hexachlorostannates then began after some time. After 3 days standing it was filtered, hydrolyzed with warm H<sub>2</sub>O and the aldehyde steam-distilled. The following p-substituted benzaldehydes were obtained in this way in excellent yields (substituent given): Me, MeO, Cl, and Br. In p-NO<sub>2</sub>- and m-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CN at 0° only the NO<sub>2</sub> group was reduced. Increasing the RCN-SnCl<sub>2</sub> ratio to 1:6 did not affect p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CN; however it led to 29% m-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHO and 61% m-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CN. Reduction of both functional groups has been achieved in neither m- nor p-nitrobenzonitrile. Generally, electron donating substituents increased the nucleophilic properties of the nitrile group and facilitated aldimine formation, and conversely. In contrast to straight-chain aliphatic nitriles, which give bisamides, branched-chain aliphatic nitriles with more than 7 C atoms (RCN-SnCl<sub>2</sub> = 1:1.1, after 8 days standing) are converted readily, but with low yields into the corresponding aldehydes, as was shown with 3-ethylenanthronitrile, 2-methylcapronitrile and 4,6,6-trimethylenanthronitrile.

IT 2570-95-8, Heptanenitrile, 4,6,6-trimethyl-  
(reduction with SnCl<sub>2</sub>)

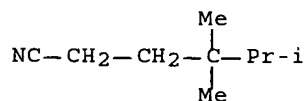
RN 2570-95-8 CAPLUS

CN Heptanenitrile, 4,6,6-trimethyl- (7CI, 9CI) (CA INDEX NAME)

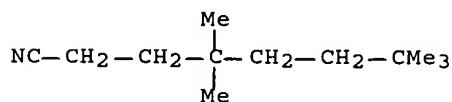




L12 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1961:17973 CAPLUS Full-text  
 DN 55:17973  
 OREF 55:3606b-d  
 TI 5-Neopentyl-5-allylbarbituric acid and related compounds. I. Preparation  
 of  $\beta$ -tert-alkylpropionic acids and derivatives  
 AU Brandstrom, Arne  
 CS Pharmacia Ltd., Uppsala, Swed.  
 SO Acta Chemica Scandinavica (1959), 13, 613-15  
 CODEN: ACHSE7; ISSN: 0904-213X  
 DT Journal  
 LA English  
 AB cf. *ibid.* 10, 1197(1956). 5-Neopentyl-5-allylbarbituric acid, a good  
 sedative, was synthesized from  $\text{ClCH}_2\text{CH}_2\text{CMe}_3$ , readily converted into 94%  
 $\text{Me}_3\text{CCH}_2\text{CH}_2\text{CN}$  (I), b5 57-9°; 93%  $\text{EtCMe}_2\text{CH}_2\text{CH}_2\text{CN}$ , b. 76-80, 91%  
 $\text{Me}_2\text{CHCMe}_2\text{CH}_2\text{CH}_2\text{CN}$ , b8 88-9°, and 80%  $\text{Me}_3\text{CCH}_2\text{CH}_2\text{CMe}_2\text{CH}_2\text{CH}_2\text{CN}$ , b8 107-10°,  
 were similarly prepared. The cyanides were hydrolyzed to 77%  $\text{Me}_3$   
 $\text{CCH}_2\text{CH}_2\text{CO}_2\text{H}$  (II), b8 104-5°, 46%  $\text{EtCMe}_2\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$ , b10 112-20°, and 50%  
 $\text{Me}_2\text{CHCMe}_2\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$ , b8 129-35°. II was also prepared by hydrogenating  
 $\beta$ -tert-butylacrylic acid over Pd-C; the Et ester of II, b8 60-2°, was  
 prepared (86% yield) by refluxing II 8 hrs. with EtOH.  
 IT 99064-65-0, Hexanenitrile, 4,4,5-trimethyl- 100247-00-5,  
 Octanenitrile, 4,4,7,7-tetramethyl-  
 (preparation of)  
 RN 99064-65-0 CAPLUS  
 CN Hexanenitrile, 4,4,5-trimethyl- (9CI) (CA INDEX NAME)



RN 100247-00-5 CAPLUS  
 CN Octanenitrile, 4,4,7,7-tetramethyl- (6CI) (CA INDEX NAME)



L12 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1952:5236 CAPLUS Full-text

DN 46:5236

OREF 46:879b-i

TI Synthesis and reactions of branched-chain hydrocarbons. I. Hydrocarbons with the 3,5,5-trimethylhexyl groups

AU Gutman, E. M.; Hickinbottom, W. J.

CS Queen Mary Coll., London

SO Journal of the Chemical Society, Abstracts (1951) 2064-7

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DT Journal

LA Unavailable

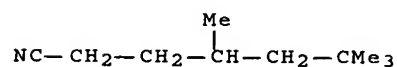
AB This series considers the reactions and properties of paraffins with a regular pattern of quaternary C atoms; this first paper deals with the possibilities and limitations of alkylmagnesium halides having quaternary C atoms for such syntheses.  $\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CH}_2\text{OH}$  (I) (144 g.) in 79 g.  $\text{C}_5\text{H}_5\text{N}$ , treated gradually (with stirring and cooling) with 125 g.  $\text{SOCl}_2$ , stirred an addnl. 20 min., gradually heated to  $110^\circ$ , and kept at that temperature 2-4 hrs. (cessation of evolution of  $\text{SO}_2$ ), gives 91%  $\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CH}_2\text{Cl}$  (II), b17  $70^\circ$ , nD25 1.4304. II is hydrolyzed very slowly by aqueous alkali; it reacts only sluggishly in ether with Mg. The Grignard reagent (III) can be prepared in 78% yield after starting the reaction with MeI. Oxidation of III gives 67% I. I (19.8 g.), 60 g. 48% HBr, and 15.6 g. concentrated  $\text{H}_2\text{SO}_4$ , refluxed 6 hrs., give 70% 1-bromo analog of II, b12  $75^\circ$ , nD20 1.4527. III from 65 g. II, 9.8 g. Mg, and 150 ml. ether, added to 14.4 g. AcOEt and refluxed, gives 78% 2,2,4,7,10,12,12-heptamethyl-7-tridecanol (IV), b9.5  $120^\circ$ , nD20 1.4512; IV and a little iodine, heated until  $\text{H}_2\text{O}$  formation ceases (0.5 hr.) and the residue refluxed 3 hrs. over Na, give a product composed largely of 2,2,4,7,10,12,12-heptamethyl-6-tridecene (V) [with some  $(\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CH}_2)_2\text{C}:\text{CH}_2$ ], b0.55  $101-3^\circ$ , nD20 1.4389-98. With  $\text{O}_3$ , 22 g. V yields HCHO, 10.3 g. 5,7,7-trimethyl-2-octanone (VI), b28  $103^\circ$ , nD20 1.4309 (semicarbazone, m.  $147.5-8.5^\circ$ ; 2,4-dinitrophenylhydrazone, m.  $80^\circ$ ), 0.6 g. b1.3  $120-34^\circ$ , and 4.6 g.  $\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CO}_2\text{H}$  (VII) (S-benzylthiuronium salt, m.  $154^\circ$ ). Hydrogenation of V in EtOH over Raney Ni at  $150^\circ/39$  atmospheric gives 79% 2,2,4,7,10,12,12-heptamethyltridecane, b0.5  $112^\circ$ , nD20 1.4437, d1919 0.7901.  $\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CH}_2\text{CN}$  (5.3 g.) and MeMgI give 1.6 g. VI. III from 19.5 g. II in ether, refluxed 3 hrs. with  $\text{CdCl}_2$ , the ether replaced by 70 ml.  $\text{C}_6\text{H}_6$ , and treated with 7.6 g.  $\text{AlCl}_3$  in 20 ml.  $\text{C}_6\text{H}_6$ , gives 6.1 g. VI. II (97.5 g.) and 78 g. KCN in 75 ml.  $\text{H}_2\text{O}$  and 170 ml. EtOH, refluxed 72 hrs., give 59.5 g. 1-cyano-3,5,5-trimethylhexane (VII), b11  $97-8^\circ$ , nD20.7 1.4294; hydrolysis of 20 g. VII by boiling 24 hrs. with alc.-aqueous NaOH, gives 19.8 g. 3,3,5-trimethyl-1-hexanecarboxylic acid, b8  $132-3^\circ$ , nD21 1.4346; S-benzylthiuronium salt, m.  $153^\circ$ ; chloride (VIIA), b22  $104^\circ$ , nD21 1.4411; amide, m.  $107^\circ$ ; Et ester (VIII), b9  $96.5^\circ$ , nD21.2 1.4254. VIII (40 g.) in 60 ml. ether, added dropwise to III from 80.5 g. II in 150 ml. ether and refluxed 1 hr., gives 60 g. 2,2,4,10,12,12-hexamethyl-7-(3,5,5-trimethylhexyl)-7-tridecanol (IX), b0.8  $176-8^\circ$ , nD20 1.4558; dehydrogenation of 40 g. IX with iodine (3 hrs. at  $200^\circ$ ) gives 31 g. 2,2,4,10,12,12-hexamethyl-7-(3,5,5-trimethylhexyl)-7-tridecene (X), b0.8  $161-2^\circ$ , nD26.4 1.4548; the action of  $\text{O}_3$  on 8.6 g. X yields 1.9 g. 2,2,4,10,12,12-hexamethyl-7-tridecanone (XI), b1.1  $124^\circ$ , nD20 1.4460 (semicarbazone, m.  $69^\circ$ ; 2,4-dinitrophenylhydrazone, m.  $39^\circ$ ), and 2.8 g. VI. Hydrogenation of X in EtOH over Raney Ni ( $180^\circ/27$  atmospheric) gives 78% 2,2,4,10,12,12-hexamethyl-7-(3,5,5-trimethylhexyl)tridecane, b0.5  $166^\circ$ , nD20 1.4558, d2020 0.8152. VIIA

(from 20.5 g. acid) and  $(\text{Me}_3\text{CCH}_2\text{CHMeCH}_2)_2\text{Cd}$  (from 31 g. II) in  $\text{C}_6\text{H}_6$  give 68% XI. III (from 32.5 g. II) and 37.6 g. AgBr, refluxed 1 hr., give 8.2 g. 2,2,4,9,11,11-hexamethyldodecane, b<sub>10</sub> 138.5°, n<sub>D20</sub> 1.4370; much olefin is formed.

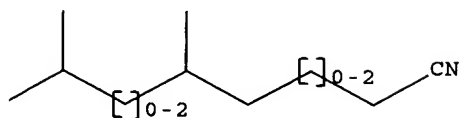
IT 2570-95-8, Heptanenitrile, 4,6,6-trimethyl-  
(preparation of)

RN 2570-95-8 CAPLUS

CN Heptanenitrile, 4,6,6-trimethyl- (7CI, 9CI) (CA INDEX NAME)



=> d l5; d his; log y  
 L5 HAS NO ANSWERS  
 L5 STR



Structure attributes must be viewed using STN Express query preparation.

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FILE 'REGISTRY' ENTERED AT 14:32:08 ON 03 MAR 2005

L1 STRUCTURE UPLOADED

L2 0 S L1

FILE 'STNGUIDE' ENTERED AT 14:33:01 ON 03 MAR 2005

FILE 'REGISTRY' ENTERED AT 14:34:22 ON 03 MAR 2005

L3 STRUCTURE UPLOADED

L4 50 S L3

L5 STRUCTURE UPLOADED

L6 25 S L5

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L9 282192 S 0/O AND 8-13/C AND 1/N

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FILE 'CAPLUS' ENTERED AT 14:38:36 ON 03 MAR 2005

L12 20 S L11

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